

Wave function of a Brownian particle

R. M. Cavalcanti*

Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106-4030

Abstract

Using the Hamiltonian of Caldirola [Nuovo Cimento **18**, 393 (1941)] and Kanai [Prog. Theor. Phys. **3**, 440 (1948)], we study the time evolution of the wave function of a particle whose classical motion is governed by the Langevin equation $m\ddot{x} + \eta\dot{x} = F(t)$. We show in particular that if the initial wave function is Gaussian, then (i) it remains Gaussian for all times, (ii) its width grows, approaching a finite value when $t \rightarrow \infty$, and (iii) its center describes a Brownian motion and so the uncertainty in the position of the particle grows without limit.

PACS numbers: 05.40.+j, 03.65.-w

Typeset using REVTeX

*Electronic address: rmc@itp.ucsb.edu

One of the starting points for the theory of the Brownian motion is the Langevin equation

$$m\ddot{x} + \eta\dot{x} + \frac{\partial V}{\partial x} = F(t), \quad (1)$$

where m is the mass of the particle, η is a damping constant, $V(x)$ is the potential acting on the particle and $F(t)$ is a Gaussian random force, obeying the relations

$$\overline{F(t)} = 0, \quad \overline{F(t)F(t')} = \phi(t - t'), \quad (2)$$

where $\phi(t)$ is a function sharply peaked at $t = 0$ and the overbar represents the average over noise.

The need to quantize such a system appears naturally when one studies, for instance, quantum electrodynamics in cavities, the low-temperature behavior of Josephson junctions or the effects of dissipation on quantum tunneling (for references, see [1,2]). In the system-plus-reservoir approach [1,2], one treats the system in which one is interested and its environment, the “reservoir,” as a closed composite system, applies the usual rules of quantization, and then eliminates the reservoir degrees of freedom.

A more phenomenological approach consists in the quantization of the Caldirola-Kanai (CK) time-dependent Hamiltonian [3],

$$H = e^{-\gamma t} \frac{p^2}{2m} + e^{\gamma t} [V(x) - F(t)x] \quad \left(\gamma \equiv \frac{\eta}{m} \right), \quad (3)$$

from which Eq. (1) results as a consequence of the Hamilton equations. Making the usual association $p = -i\partial/\partial x$ (in units such that $\hbar = 1$), one then obtains the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(x, t) = \left\{ -\frac{e^{-\gamma t}}{2m} \frac{\partial^2}{\partial x^2} + e^{\gamma t} [V(x) - F(t)x] \right\} \psi(x, t). \quad (4)$$

This approach has been severely criticized by some authors [4], but Caldirola and Lugiatto [5] have shown that, in the case of the damped harmonic oscillator with a stochastic force, it gives the the same results as the more orthodox approach based on a master equation derived by elimination of the degrees of freedom of the thermal reservoir. Their analysis can be generalized for an arbitrary potential $V(x)$, if one uses the Caldeira-Leggett model [1] to describe the interaction of the particle with its environment. One can then derive a quantum-mechanical Langevin equation for the position operator of the particle with an operator-valued stochastic force [6]. The CK Hamiltonian can then be viewed as an effective one-particle Hamiltonian that, through the Heisenberg equations of motion for x and p , generates the Langevin equation for x . One should note, however, that because $F(t)$ is an operator in the Hilbert space of the environment, the wave function $\psi(x, t)$ is also an operator in that space since it is a functional of $F(t)$. Therefore, in order to obtain expectation values of operators defined in the Hilbert space of the particle, one must know not only the wave function $\psi(x, t)$ [7], but also the state of the reservoir, as specified by its density operator, which in turn determines the noise correlation function $\phi(t)$. [In practice, if one is not interested in short-time effects, one can assume a white noise, i.e., $\phi(t) = D \delta(t)$, where D is a

temperature-dependent coefficient determined in accordance with the fluctuation-dissipation theorem.] Interpreted this way, the Caldirola-Kanai approach to the quantum Brownian motion is akin to the quantum state diffusion picture proposed by Gisin and Percival [8], in which a master equation for the density operator ρ is replaced with a stochastic equation of motion for the state vector $|\psi\rangle$; the former is then recovered by averaging $|\psi\rangle\langle\psi|$ over the fluctuations. In what follows, we shall illustrate these ideas by studying the evolution of a wave packet in the case $V = 0$.

In order to solve Eq. (4) (with $V = 0$), we first make the change of variable

$$\tau(t) = \frac{1}{\gamma} (1 - e^{-\gamma t}). \quad (5)$$

Equation (4) then becomes

$$i \frac{\partial}{\partial \tau} \psi(x, \tau) = \left[-\frac{1}{2m} \frac{\partial^2}{\partial x^2} - f(\tau)x \right] \psi(x, \tau), \quad (6)$$

where

$$f(\tau) = e^{2\gamma t} F(t) = \frac{F(-\gamma^{-1} \ln(1 - \gamma\tau))}{(1 - \gamma\tau)^2}. \quad (7)$$

Equation (6) is the Schrödinger equation of a particle in a time-dependent electric field, for which solutions can be found the form of plane waves [9]. In fact,

$$\psi(x, \tau) = N e^{ip(\tau)x - i\alpha(\tau)} \quad (8)$$

is a solution of Eq. (6) provided $p(\tau)$ and $\alpha(\tau)$ satisfy

$$\frac{dp}{d\tau} = f(\tau), \quad \frac{d\alpha}{d\tau} = \frac{p^2}{2m}. \quad (9)$$

The solutions of these equations (and the corresponding wave functions) can be labeled by the initial value of $p(\tau)$, which we denote by k ,

$$p_k(\tau) = k + \int_0^\tau f(\tau') d\tau' \equiv k + I(\tau), \quad (10a)$$

$$\begin{aligned} \alpha_k(\tau) &= \frac{1}{2m} \left[k^2 \tau + 2k \int_0^\tau I(\tau') d\tau' + \int_0^\tau I^2(\tau') d\tau' \right] \\ &\equiv \frac{k^2 \tau}{2m} + k f_1(\tau) + f_2(\tau). \end{aligned} \quad (10b)$$

[The initial value of $\alpha(\tau)$ can be absorbed in the normalization constant N and so without lack of generality, we may take $\alpha(0) = 0$.] With $N = (2\pi)^{-1/2}$, one can easily verify that

$$\int_{-\infty}^{\infty} \psi_k^*(x, \tau) \psi_{k'}(x, \tau) dx = \delta(k - k'), \quad (11a)$$

$$\int_{-\infty}^{\infty} \psi_k(x, \tau) \psi_k^*(x', \tau) dk = \delta(x - x'). \quad (11b)$$

The second identity allows one to write the propagator as

$$G(x, t|x', t') = \int_{-\infty}^{\infty} \psi_k(x, \tau) \psi_k^*(x', \tau') dk, \quad (12)$$

where $\tau = \tau(t)$, $\tau' = \tau(t')$.

Using the above result, let us investigate the time evolution of the Gaussian wave packet

$$\psi(x, 0) = (2\pi\sigma^2)^{-1/4} e^{-x^2/4\sigma^2}. \quad (13)$$

Performing the integration over k in Eq. (12), one finds

$$G(x, t|x', 0) = \sqrt{\frac{m}{2\pi i\tau}} \exp \left\{ \frac{im[x - x' - f_1(\tau)]^2}{2\tau} + iI(\tau)x - if_2(\tau) \right\}, \quad (14)$$

so that

$$\begin{aligned} \psi(x, t) &= \int_{-\infty}^{\infty} G(x, t|x', 0) \psi(x', 0) dx' \\ &= (2\pi)^{-1/4} \left(\sigma + \frac{i\tau}{2m\sigma} \right)^{-1/2} \exp \left\{ -\frac{m[x - f_1(\tau)]^2}{4m\sigma^2 + 2i\tau} + iI(\tau)x - if_2(\tau) \right\}. \end{aligned} \quad (15)$$

The probability density is then given by

$$|\psi(x, t)|^2 = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp \left\{ -\frac{[x - f_1(\tau)]^2}{2\sigma^2(t)} \right\}, \quad (16)$$

where

$$\sigma(t) = \sqrt{\sigma^2 + \frac{\tau^2(t)}{4m^2\sigma^2}}. \quad (17)$$

The spreading of the wave packet is the same one found in [6,10] taking into account only the dissipation.

At first sight this result may seem paradoxical: Even in the presence of a fluctuating force, the uncertainty in position

$$(\Delta x)_{qu} \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sigma(t) \quad (18)$$

tends to a finite value when $t \rightarrow \infty$. However, it should be noted that the above quantity measures the uncertainty in the position of the particle with respect to the “center of mass” of the wave packet, $\langle x(t) \rangle$, which cannot be determined precisely: According to Ehrenfest theorem, $\langle x(t) \rangle$ satisfies Eq. (1) and so describes a Brownian motion. Therefore, there is a “classical” uncertainty in the position of the center of the wave packet that, in the case of a white noise, is given by [11]

$$(\Delta x)_{cl} \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{D}{\eta^2} [t - \gamma^{-1}(1 - e^{-\gamma t})]}, \quad (19)$$

which, in contrast with the “quantum” uncertainty in the position of the particle, does not “freeze” when $t \rightarrow \infty$.

The above definitions of quantum and classical uncertainties are somewhat artificial since they cannot be directly compared with experiment. (This would require not only an ensemble of particles with the same initial state, which one could possibly manage to prepare, but also an ensemble of reservoirs in the same microstate.) As argued before, the natural definition of the expectation value of an operator \mathcal{O} (i.e., the one that can be compared with experiment) is given by $\overline{\langle \mathcal{O} \rangle}$ and so the uncertainty in the position of the particle is given by

$$\Delta x \equiv \sqrt{\overline{\langle x^2 \rangle} - \overline{\langle x \rangle}^2} = \sqrt{(\Delta x)_{qu}^2 + (\Delta x)_{cl}^2}. \quad (20)$$

In conclusion, I would like to emphasize that the whole point of the above exercise is to show that, *provided fluctuation effects are properly taken into account*, the CK approach to the quantum Brownian motion can give the same results as the more conventional approaches based on master equations or influence functionals.

I thank L. Davidovich and C. A. A. de Carvalho for a critical reading of this paper. This work was supported by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and, in part, by the National Science Foundation under Grant No. PHY94-07194.

REFERENCES

- [1] A. O. Caldeira and A. J. Leggett, *Physica A* **121**, 587 (1983).
- [2] U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 1993).
- [3] P. Caldirola, *Nuovo Cimento* **18**, 393 (1941); E. Kanai, *Prog. Theor. Phys.* **3**, 440 (1948).
- [4] Most of these criticisms are rebutted (properly, in my opinion) by V. J. Menon, N. Chanana and Y. Singh, *Prog. Theor. Phys.* **98**, 321 (1997).
- [5] P. Caldirola and L. A. Lugiato, *Physica A* **116**, 248 (1982).
- [6] C. P. Sun and L. H. Yu, *Phys. Rev. A* **51**, 1845 (1995).
- [7] This is another way to say that a Brownian particle (or, more generally, an open system) does not have a wave function. See L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 3rd. ed. (Pergamon, Oxford, 1977), §14.
- [8] N. Gisin and I. C. Percival, *J. Phys. A* **25**, 5677 (1992).
- [9] S. Fallieros and J. L. Friar, *Am. J. Phys.* **50**, 1001 (1992).
- [10] R. W. Hasse, *J. Math. Phys.* **16**, 2005 (1975).
- [11] F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965), Chap. 15. [It should be emphasized that this result is derived under the assumption of a white-noise. For instance, in Sec. 7 of Ref. [1] the authors show that when $T \rightarrow 0$, $(\Delta x)^2 \sim \ln t$ when $t \rightarrow \infty$, in contrast with the behavior predicted by Eq. (19). This discrepancy occurs because in their model for the reservoir the noise becomes “colored” when $T \rightarrow 0$.]